

# Microcanonical distributions for quantum systems

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**Abstract.** A new theory of the quantum microcanonical distribution is presented, based on the geometric formulation of quantum mechanics. We consider the case of a quantum system for which the associated Hilbert space is finite-dimensional. The space of pure quantum states, for the given quantum system, is a symplectic manifold with a Hamiltonian structure. For any specified value of the energy, the natural microcanonical distribution on this symplectic manifold is given by a uniform measure on the corresponding level surface of the expectation value of the Hamiltonian operator. The properties of this distribution, and the associated density matrix, are investigated in some detail. In particular, a general closed-form expression for the density of states is obtained, valid both for degenerate and nondegenerate energy spectra. This result is applied to a variety of examples, for which the behaviour of the state density, as well as the relation between energy and temperature, are determined. We show that the microcanonical equilibrium states predicted by our theory can exhibit second-order phase transitions. (11 October 2005)

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## 1. Introduction

In classical statistical mechanics the foundational role of the microcanonical distribution is well established. Indeed, investigations in classical statistical mechanics can be divided broadly into two types: those investigations that assume that the equilibrium of an isolated classical system with a definite total energy can be described by the microcanonical distribution function, and proceed on the basis of this assumption; and those that try to establish this postulate as a fact that is derivable from more primitive considerations (e.g., from kinetic theory, or ergodic theory). The situation in quantum statistical physics, however, is different: in most treatments the quantum microcanonical distribution is given only a brief discussion, leading, by way of loose arguments, to the familiar expression for the microcanonical density matrix (see, e.g., [12, 18, 20, 25, 27, 29, 30]). The matter is complicated further by the fact that the quantum microcanonical distribution is usually only defined for a system with a total energy in some specified band, rather than with a sharp total energy. The result of

this is that much of the mathematical beauty and physical generality of the classical statistical theory is lost, and one is left with a conceptual foundation for the equilibrium physics of large quantum systems that is in many respects less than satisfactory.

There has, however, been one modern development in quantum theory that may allow for a way forward with this issue. This is the geometric approach to quantum mechanics proposed by Kibble [17] and others. Kibble's observation was that the space of pure states of a quantum system, when regarded as a complex projective space with the Fubini-Study metric, has natural structure of a symplectic manifold. The expectation of the Hamiltonian operator, when taken for each pure state, then defines a Hamiltonian function on this manifold, endowing it with a nondegenerate Hamiltonian structure. The picture is completed with the remark that the dynamical trajectories generated by this Hamiltonian structure, for a given initial condition on the state space, turn out to be given by the Schrödinger evolution. Thus a more or less entirely satisfactory description of quantum theory can be formulated in the language of classical mechanics—that is to say, classical mechanics in the very general modern sense, which has symplectic geometry as its foundation, as represented, e.g., in [1, 3, 21]. For further details of the geometrical approach to quantum theory, see, e.g., [2, 4, 5, 8, 10, 13].

The particular feature of classical statistical mechanics that makes that framework hold together so satisfactorily is that it is, in essence, a theory of probability distributions on symplectic manifolds. The standard Gibbsian distributions—the microcanonical distribution, the canonical distribution, the grand canonical distribution, and the pressure-temperature distribution—emerge as special distributions that are related in specific ways to the underlying symplectic manifold and its Hamiltonian structure. But since the space of pure quantum states is also a symplectic manifold with a Hamiltonian structure, this suggests the possibility of a new foundation for quantum statistical mechanics—namely, as a theory of probability distributions on the space of pure quantum states.

In this paper we consider, in particular, the construction and application of what we shall call the symplectic quantum microcanonical (SQM) distribution. This distribution is defined as follows. By an energy surface in a space of pure quantum states, we mean any surface over which the expectation of the Hamiltonian operator takes a level value. For example, in the case of a two-dimensional Hilbert space, the space of pure states is a sphere (the space of rays through the origin in the Hilbert space). If the Hamiltonian is nondegenerate, there are two eigenstates, corresponding, say, to the north and south poles. The energy surfaces are the circles of constant latitude. In higher-dimensional quantum systems the energy surfaces typically have an extremely complex and rich structure (see [5]). By an SQM distribution for a quantum system with energy  $E$ , we mean a probability distribution, on the space of pure quantum states, whose support lies on the energy surface  $\mathcal{E}_E$  with energy  $E$ , and that is uniform on that surface. The density matrix induced by such a distribution—which we call the SQM state—turns out to be different, in rather subtle ways, from the density matrix arising in the more familiar treatments, thus raising the possibility that not only might we be able

to improve the conceptual foundations of quantum statistical mechanics through its consideration, but additionally we may be able to put the new statistical theory to the test. For this we would require the specification of a class of physical systems for which the SQM distribution would constitute a likely candidate for the characterisation of an equilibrium configuration. With this goal in mind, in the present paper we carry out an investigation of the properties of this distribution.

The paper is organised as follows. In §2 we review the formulation of quantum theory in terms of the symplectic geometry of the space of pure states, as described, e.g., in [2, 4, 5, 6, 8, 13, 17] and references cited therein. When the trajectory of a wave function is projected from Hilbert space  $\mathcal{H}$  to the space  $\mathcal{P}$  of pure states (rays through the origin of  $\mathcal{H}$ ), the Schrödinger equation on  $\mathcal{H}$  reduces to Hamilton's equation on  $\mathcal{P}$ . More precisely,  $\mathcal{P}$  has a natural symplectic structure; and the Schrödinger trajectories, when projected onto  $\mathcal{P}$ , are the integral curves of the Hamiltonian vector field obtained by taking the symplectic gradient of the function on  $\mathcal{P}$  defined by the expectation of the Hamiltonian operator. As a consequence, the formulation of quantum mechanics on  $\mathcal{P}$  provides a natural environment in which one can study the quantum analogues of issues and phenomena arising in the context of Hamiltonian mechanics, such as those associated with ergodicity conditions or the construction of equilibrium distributions. For example, the dynamical approach to microcanonical equilibrium introduced by Rugh [26] for classical systems can be seen to apply in the quantum regime.

In §3 we introduce the natural microcanonical density of states that follows from the symplectic microcanonical postulate, together with the associated microcanonical density matrix. We provide a physical motivation for the introduction of the SQM state by considering the properties of an idealised quantum gas. In §4 we derive a general integral representation for the density of states, expressed in terms of the energy eigenvalues. We then perform the integration explicitly in the case for which the energy spectrum is nondegenerate. Finally, the analysis for the nondegenerate spectrum is extended in such a way as to allow us to obtain an analogous expression for the density of states associated with a system having any number of degeneracies.

As an illustration, the properties of a system having an equally-spaced energy spectrum are studied in §5. In this example we study the relation between the energy and the temperature in some detail, which we plot for a number of different situations. We also plot the corresponding specific heats of these systems, which exhibit an interesting singular behaviour. A simple procedure for rescaling the energy shows that, as the dimensionality of the Hilbert space increases, the system becomes more and more likely to take the intermediate energy value  $\frac{1}{2}(E_{\max} + E_{\min})$ , where  $E_{\max}$  and  $E_{\min}$  are, respectively, the largest and the smallest energy eigenvalues. To study the convergence of the distribution numerically, we consider a system whose spectrum is equally spaced and lies in the range  $[0, 1]$ . For this system we compute the Hellinger distance between the density of states associated with an  $n$ -level system and an  $(n + 1)$ -level system for  $n = 2, 3, \dots$ . The result of the computation establishes that the logarithmic plot of the relative distances of the distributions against the Hilbert space dimensionality lies on a

straight line with gradient  $-2$ . Finally we study the properties of systems having other nondegenerate spectra. We show numerically that there is an approximate symmetry relation that holds between a system having the spectrum  $E_k \sim k^m$  and a system having the spectrum  $E_k \sim k^{1/m}$ , where  $m$  is a constant.

## 2. Quantum phase space as a basis for quantum statistical mechanics

Our goal in this paper is to gain some insight into the nature of the equilibrium states of isolated quantum systems. We shall use the Hamiltonian formulation of quantum mechanics advocated by Kibble [17], and others, as our starting point. The advantage of the Kibble approach, in the present context, is that it presents quantum mechanics in such a way that the techniques of symplectic geometry can be brought into play. More specifically, by use of the Kibble formalism we can take advantage of the fact the the space of pure quantum states is a symplectic manifold with a natural Hamiltonian structure. This point is crucial in our analysis of the foundations of quantum statistical mechanics, and is what distinguishes it from the more traditional treatments. In particular, we are able to apply concepts arising in the corresponding classical theory of equilibrium as outlined, for example, in [9, 15, 28].

Consider a quantum system whose pure states can be represented by the elements of a complex Hilbert space  $\mathcal{H}$  of dimension  $n + 1$ . We denote by  $Z^\alpha$  a typical element of  $\mathcal{H}$ , where  $\alpha$  runs over the range  $\alpha = 0, 1, \dots, n$ . The Hamiltonian of the system will be denoted  $H_\beta^\alpha$ , and the expectation value of  $H_\beta^\alpha$  in the state represented by  $Z^\alpha$  is

$$\langle H \rangle = \frac{\bar{Z}_\alpha H_\beta^\alpha Z^\beta}{\bar{Z}_\gamma Z^\gamma}, \quad (1)$$

where  $\bar{Z}_\alpha$  is the complex conjugate of  $Z^\alpha$ . The space  $\mathcal{H}$  carries an irrelevant complex degree of freedom given by the overall scale of the state vector. This follows from the fact that the expectation value of a physical observable is invariant under the scale transformation  $Z^\alpha \rightarrow \lambda Z^\alpha$ , where  $\lambda \in \mathbb{C} - \{0\}$ . It is useful in some applications to eliminate this degree of freedom by considering the space of equivalence classes under the relation  $\lambda Z^\alpha \sim Z^\alpha$  for  $\lambda \in \mathbb{C} - \{0\}$ . This is the space of rays through the origin of  $\mathcal{H}$ , otherwise known as the projective Hilbert space  $\mathcal{P}$  of complex dimension  $n$ .

It is well known now that quantum theory, when formulated on the projective space  $\mathcal{P}$ , admits a natural representation in terms of the mathematical structure of Hamiltonian mechanics. This can be seen as follows.

The first step is to regard the projective space  $\mathcal{P}$  as a real manifold  $\Gamma$  of dimension  $2n$ , letting  $x^a$  ( $a = 1, 2, \dots, 2n$ ) denote a typical point in  $\Gamma$ . Each point  $x^a \in \Gamma$  represents a ray in the Hilbert space  $\mathcal{H}$ . In this way we can regard the expression for the expectation value (1) as determining a real-valued function  $H(x)$  on  $\Gamma$ .

The space of pure quantum states for the given system, when regarded as the real even-dimensional manifold  $\Gamma$ , comes endowed with a natural symplectic structure, given by a nondegenerate two-form  $\omega_{ab}$ . The dynamical laws governing the trajectories

of quantum states, given by the Schrödinger equation on  $\mathcal{H}$ , can be represented on  $\Gamma$  in Hamiltonian form as follows:

$$\frac{1}{2}\hbar\omega_{ab}\frac{dx^b}{dt} = \nabla_a H(x). \quad (2)$$

The space  $\Gamma$  is thus a symplectic manifold upon which the evolution of a quantum state is governed by Hamilton's equations, which in the language of symplectic geometry take the form (2). We can therefore regard  $\Gamma$  as the quantum analogue of a classical phase space. The state space of any quantum system is in possession of this structure—it is, so to speak, part of the basic setup of quantum theory. Given the prominent role of the geometry of the phase space in classical statistical mechanics, it is natural to enquire whether the symplectic structure of the quantum phase space also has a role to play in quantum statistical mechanics. Indeed, it would be an odd state of affairs if it did not; but the historical development of quantum statistical mechanics has been such that the main treatment of the subject preceded the introduction of symplectic methods in quantum theory. Therefore in what follows we propose to formulate a theory of equilibrium states in quantum statistical mechanics making use of the natural symplectic geometry of  $\Gamma$ .

### 3. The microcanonical distribution

#### 3.1. Definition of the state density

We begin this section by considering the foliation of the quantum phase space  $\Gamma$  by level surfaces of the Hamiltonian function  $H(x)$ . This is given by a family of hypersurfaces  $\{\mathcal{E}_E\}$ ,  $E \in [E_{\min}, E_{\max}]$ , determined by level values  $H(x) = E$ . The structure of the typical energy surface in quantum mechanics is intricate, even for a system described by low-dimensional Hilbert space. In particular, as  $E$  varies in the range  $[E_{\min}, E_{\max}]$  both the dimensionality and the topology of the associated energy surfaces can change. An example can be found in Ref. [5], in which the structures of the energy surfaces for a three-level system are described.

Given this foliation, the ‘number’ of microscopic quantum mechanical configurations (pure states) with expected energy in the small range  $E$  and  $E + \Delta E$  is  $\Omega(E)\Delta E$ , where the density of states  $\Omega(E)$  for energy  $E$  is an expression of the form

$$\Omega(E) = \int_{\mathcal{E}_E} \frac{\nabla_a H d\sigma^a}{\nabla_b H \nabla^b H}. \quad (3)$$

Here the natural vector-valued  $(2n - 1)$ -form  $d\sigma^a$  on  $\Gamma$  is defined by

$$d\sigma^a = g^{ab} \epsilon_{bc\dots d} dx^c \cdots dx^d, \quad (4)$$

where  $\epsilon_{bc\dots d}$  denotes the totally skew tensor with  $n$  indices, and  $g^{ab}$  is the inverse of the natural Riemannian metric  $g_{ab}$  on  $\Gamma$  (which is the Fubini-Study metric [19]). The metric  $g_{ab}$  is compatible with the symplectic structure  $\omega_{ab}$  in the sense that  $\nabla_a \omega_{bc} = 0$ , where  $\nabla_a$  is the unique torsion-free covariant derivative operator on  $\Gamma$  satisfying  $\nabla_a g_{bc} = 0$ . It is a remarkable feature of the quantum phase space that it has both a natural Riemannian

metric and a compatible symplectic structure; as we indicated above, these elements can be regarded as part of the natural geometry of any quantum system.

In the case of an isolated quantum system with energy in the range from  $E$  to  $E + \Delta E$ , we can adopt the notion of the microcanonical distribution as it is usually defined in classical statistical mechanics (see, e.g., [12]), and identify the entropy of the system by use of the Boltzmann relation

$$S(E) = k_B \ln(\Omega(E)\Delta E), \quad (5)$$

where  $k_B$  is Boltzmann's constant. Here we are implicitly assuming what might be called the *symplectic quantum microcanonical postulate*, which in our scheme asserts that *for an isolated system in equilibrium all states on a given energy surface in the quantum phase space are equally probable*. As a consequence, the temperature  $T$  of such a system is determined by the relation

$$\frac{1}{T} = \frac{dS(E)}{dE}. \quad (6)$$

Thus for an isolated quantum system with energy  $E$ , we propose that the equilibrium configuration is given by a uniform distribution on the energy surface  $\mathcal{E}_E$ , with entropy  $S(E)$  and temperature  $T(E)$ , as given above. The corresponding probability measure on the quantum phase space, which we call the SQM distribution, is given by

$$\mu_E(x) = \frac{1}{\Omega(E)} \delta(H(x) - E), \quad (7)$$

where

$$\Omega(E) = \int_{\Gamma} \delta(H(x) - E) dV. \quad (8)$$

Here  $dV$  is the volume element on  $\Gamma$ . Thus the equilibrium state of an isolated quantum system with total energy  $E$  can be characterised by the distribution  $\mu_E(x)$  on  $\Gamma$ .

### 3.2. Physical motivation of the SQM postulate

One might ask, of course, what it means for an isolated quantum system to have energy  $E$ , where  $E$  lies in the continuous range  $[E_{\min}, E_{\max}]$ , if the energy levels of the Hamiltonian are restricted to a finite, discrete set of eigenvalues  $\{E_i\}_{i=0,1,\dots,n}$ . And what does it mean for such an 'isolated' system to be 'in equilibrium'? We address these issues with the following remarks.

In physics the notion of 'equilibrium' is a big idea—there is no one-size-fits-all definition. In specific situations, however, the idea can often be given a concrete meaning. We therefore examine the following situation. Suppose we consider a large number of copies of the given quantum system, say  $N$  copies, and we envisage these as forming a 'quantum gas'. We write  $\hat{H}_{\text{total}}$  for the Hamiltonian of the composite system (i.e., the gas) as a whole, and  $\hat{H}_i$  ( $i = 1, 2, \dots, N$ ) for the Hamiltonians of the individual constituents of the gas. We assume that the interactions between the constituents are very weak, and hence that to a good approximation we have  $\hat{H}_{\text{total}} = \sum_{i=1}^N \hat{H}_i$ .

We also assume that the various constituents are to a good approximation independent. This means that the wave function for the composite system is, again to a good approximation, given by a product of constituent wave functions. Thus, for independence we assume that the support of the composite state lies on the Segré embedding (see [5]) of the product of the pure state manifolds for the various constituents in the large state manifold of the composite system. In this sense, each of the constituents is, approximately, isolated. (For simplicity we ignore issues associated with Bose and Fermi statistics.)

Let us suppose that the energy of the composite system is fixed, approximately, at some value  $E_{\text{total}}$ . More specifically, let us assume that  $\langle \hat{H}_{\text{total}} \rangle = E_{\text{total}}$ , and that  $N$  is very large. It follows that  $\sum_{i=1}^N \langle \hat{H}_i \rangle = E_{\text{total}}$ . Now consider the result of a hypothetical measurement of the energy of one of the constituents. In equilibrium we would expect that, owing to the effects of the weak interactions between the constituents, the state of each constituent should be such that, on average, the result of an energy measurement should be the same. That is to say, in equilibrium, the state of each constituent should be such that the expectation value of the energy is the same for each constituent. Therefore, writing  $E = N^{-1}E_{\text{total}}$ , we conclude that in equilibrium the gas must have the property that  $\langle \hat{H}_i \rangle = E$  for  $i = 1, 2, \dots, N$ . In other words, the state of each constituent must lie on the energy surface  $\mathcal{E}_E$  in the pure state manifold for that particular constituent. Since  $N$  is large, this will in turn ensure that the uncertainty in the total energy of the composite system, as a fraction of the expectation of the total energy, will be vanishingly small. More specifically, it follows by an application of the Chebyshev inequality that

$$\text{Prob} \left[ \frac{|\hat{H}_{\text{total}} - E_{\text{total}}|}{|E_{\text{total}}|} > x \right] \leq \frac{1}{Nx^2} \frac{\langle (\hat{H}_i - \langle \hat{H}_i \rangle)^2 \rangle}{\langle \hat{H}_i \rangle^2}, \quad (9)$$

for any choice of  $x > 0$ .

We observe that, as a matter of convenience, we can describe the distribution of the various constituent pure states, on their respective energy surface, as if we were considering a probability distribution on the energy surface  $\mathcal{E}_E$  of a single constituent. In reality, of course, we have a large number of approximately independent constituents; but owing to the fact that the respective state spaces are isomorphic we can represent the behaviour of the aggregate system with the specification of a probability measure on the energy surface of a single ‘representative’ constituent. This enables us to simplify the description of the composite system by referring to a distribution of states on the quantum phase space of a single constituent. (The consideration of distributions on the space of pure states as a basis for the foundations of quantum statistical mechanics is also pursued, e.g., in [14] and [16].)

We can ask, what does this distribution on  $\mathcal{E}_E$  look like? In equilibrium, evidently, the distribution must be uniform on  $\mathcal{E}_E$ . One way to see this is as follows. It is reasonable to suppose that the equilibrium distribution, whatever it may be, maximises an appropriate entropy functional on the set of possible probability distributions on  $\mathcal{E}_E$ . Writing  $dV$  for the volume element on  $\mathcal{E}_E$ , one can consider a general entropy functional

of the form  $\int_{\mathcal{E}_E} \Phi(\rho(x))dV$  where  $\rho(x)$  is a density function with support on  $\mathcal{E}_E$ . For an entropy functional we require  $\Phi$  to be concave [7], and we have the normalisation constraint  $\int_{\mathcal{E}_E} \rho(x)dV = 1$ . A standard argument then shows that  $\rho(x)$  must be constant over  $\mathcal{E}_E$ . Alternatively, from a physical point of view we can argue that the constituents of the gas approach their equilibrium configuration in two different ways. On the one hand, weak exchanges of energy result in all the states eventually settling on or close to the energy surface  $\mathcal{E}_E$ ; on the other hand, the continued weak interactions will induce an effectively random perturbation in the Schrödinger dynamics of each constituent, causing it to undergo a Brownian motion on  $\mathcal{E}_E$  that in the long run induces uniformity in the distribution on  $\mathcal{E}_E$ .

We conclude that for the particular ‘quantum gas’ that we have been considering the equilibrium configuration can be represented by a uniform measure on an energy surface of an isolated representative constituent of the gas. We call this measure the symplectic quantum microcanonical distribution.

### 3.3. The microcanonical density matrix

Returning to the analysis of the state density, we note that it is a straightforward exercise to show that starting from the definition (8) of the density of states  $\Omega(E)$  we can deduce the integral formula (3). This can be seen as follows. At each point  $x \in \Gamma$  such that  $\nabla_a H(x) \neq 0$ , the volume element on  $\Gamma$  can be written as a product  $dV = dN d\sigma$ , where the  $(n - 1)$ -form  $d\sigma$  defined by

$$d\sigma = \frac{\nabla^a H \epsilon_{ab\dots c} dx^b \dots dx^c}{\sqrt{\nabla_d H \nabla^d H}} \quad (10)$$

is the volume element on the energy surface passing through  $x$ , and

$$dN = \frac{\nabla_a H dx^a}{\sqrt{\nabla_b H \nabla^b H}}. \quad (11)$$

On the other hand, as a consequence of the relation  $dH = \nabla_a H dx^a$  we observe that

$$dN = \frac{dH}{\sqrt{\nabla_a H \nabla^b H}}. \quad (12)$$

Substituting this expression into (8) we obtain

$$\begin{aligned} \Omega(E) &= \int_{\Gamma} \delta(H(x) - E) dV \\ &= \int_{\Gamma} \delta(H(x) - E) \frac{d\sigma dH}{\sqrt{\nabla_a H \nabla^b H}} \\ &= \int_{\mathcal{E}_E} \frac{d\sigma}{\sqrt{\nabla_b H \nabla^b H}} \\ &= \int_{\mathcal{E}_E} \frac{\nabla^a H \epsilon_{ab\dots c} dx^b \dots dx^c}{\nabla_d H \nabla^d H}, \end{aligned} \quad (13)$$

which agrees with expression (3).

A general measurable function  $F(x)$  on  $\Gamma$  represents a nonlinear observable in the sense of Mielnik [22], Kibble [17], and Weinberg [31]. The usual linear observables of

quantum mechanics correspond to the situation for which  $F(x)$  can be represented as the expectation of a Hermitian operator. In either case, for each value of  $x$  we interpret  $F(x)$  as the conditional expectation  $\langle F \rangle_x$  of the observable  $F$  in the pure state  $x$ . The unconditional expectation of  $F$  in the microcanonical state is given by

$$\langle F \rangle_E = \int_{\Gamma} F(x) \mu_E(x) dV. \quad (14)$$

In the case of a linear observable we have

$$F(x) = F_{\alpha}^{\beta} \Pi_{\beta}^{\alpha}(x), \quad (15)$$

where

$$\Pi_{\beta}^{\alpha}(x) = \frac{\bar{Z}_{\beta} Z^{\alpha}}{\bar{Z}_{\gamma} Z^{\gamma}} \quad (16)$$

is the projection operator onto the state vector  $Z^{\alpha}(x)$  corresponding to the pure state  $x \in \Gamma$ . The unconditional expectation in the state  $\mu_E(x)$  is therefore

$$\langle F \rangle_E = F_{\alpha}^{\beta} \mu_{\beta}^{\alpha}(E), \quad (17)$$

where the SQM density matrix  $\mu_{\beta}^{\alpha}(E)$ , parameterised by  $E$ , is defined by

$$\mu_{\beta}^{\alpha}(E) = \int_{\Gamma} \Pi_{\beta}^{\alpha}(x) \mu_E(x) dV. \quad (18)$$

It follows immediately that  $H_{\alpha}^{\beta} \mu_{\beta}^{\alpha}(E) = E$ .

Let  $W(E)$  denote the total phase space volume of states such that  $H(x) \leq E$ . The density matrix  $\mu_{\beta}^{\alpha}(E)$  can be calculated explicitly by use of the following ‘variation-of-parameters’ formula:

$$\mu_{\beta}^{\alpha}(E) = - \left( \frac{dW(E)}{dE} \right)^{-1} \frac{\partial W(E)}{\partial H_{\alpha}^{\beta}}. \quad (19)$$

This representation can be verified as follows. From the definition of  $W(E)$  we can write

$$W(E) = \int_{-\infty}^E \int_{\Gamma} \delta(H_{\alpha}^{\beta} \Pi_{\beta}^{\alpha}(x) - u) dV du, \quad (20)$$

and hence

$$\begin{aligned} \frac{\partial W(E)}{\partial H_{\alpha}^{\beta}} &= \int_{-\infty}^E \int_{\Gamma} \Pi_{\beta}^{\alpha}(x) \delta'(H_{\alpha}^{\beta} \Pi_{\beta}^{\alpha}(x) - u) dV du \\ &= \int_{\Gamma} \Pi_{\beta}^{\alpha}(x) \left( \int_{-\infty}^E \delta'(H_{\alpha}^{\beta} \Pi_{\beta}^{\alpha}(x) - u) du \right) dV \\ &= - \int_{\Gamma} \Pi_{\beta}^{\alpha}(x) \delta(H_{\alpha}^{\beta} \Pi_{\beta}^{\alpha}(x) - E) dV \\ &= - \Omega(E) \int_{\Gamma} \Pi_{\beta}^{\alpha}(x) \mu_E(x) dV \\ &= - \Omega(E) \mu_{\beta}^{\alpha}(E). \end{aligned} \quad (21)$$

On the other hand, clearly  $dW(E)/dE = \Omega(E)$ , and thus we obtain (19).

## 4. Calculating the density of states

### 4.1. A general integral representation

As defined in equation (8) above, the density of states is given by the volume integral over  $\Gamma$  of a delta-function having support on the energy surface  $\mathcal{E}_E$ . Our objective is to perform the relevant integration explicitly for a generic Hamiltonian, and obtain a representation for  $\Omega(E)$  in terms of the energy eigenvalues.

We find it convenient to pursue the calculation by lifting the integration from the phase space  $\Gamma$  to the Hilbert space  $\mathcal{H}$ , imposing the constraint that the norm of the Hilbert space vector  $Z^\alpha$  is unity. Therefore, we write the expression (8) in the following form:

$$\Omega(E) = \frac{1}{\pi} \int_{\mathbb{C}^{n+1}} \delta(\bar{Z}_\alpha Z^\alpha - 1) \delta\left(\frac{\bar{Z}_\alpha H_\beta^\alpha Z^\beta}{\bar{Z}_\gamma Z^\gamma} - E\right) d^{n+1} \bar{Z} d^{n+1} Z. \quad (22)$$

The additional factor of  $\pi$  arises from the superfluous phase integration in (22). By use twice of the integral representation

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\lambda x} d\lambda \quad (23)$$

we deduce that

$$\begin{aligned} \Omega(E) &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} e^{i(\lambda+\nu E)} \\ &\quad \times \int_{\mathbb{C}^{n+1}} \exp\left[-i(\lambda \bar{Z}_\alpha Z^\alpha + \nu H_\beta^\alpha \bar{Z}_\alpha Z^\beta)\right] d^{n+1} \bar{Z} d^{n+1} Z. \end{aligned} \quad (24)$$

We observe that we can diagonalise the Hamiltonian by unitary transformation without affecting any of the terms in (24) on account of the fact that every ‘ket’ vector  $Z^\alpha$  is coupled to a corresponding ‘bra’ vector  $\bar{Z}_\alpha$ . Therefore, the density of states can be written in the form

$$\begin{aligned} \Omega(E) &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{i(\lambda+\nu E)} \\ &\quad \times \int_{\mathbb{C}^{n+1}} d^{n+1} \bar{Z} d^{n+1} Z \exp\left(-i \sum_{l=0}^n (\lambda + \nu E_l) \bar{Z}_l Z^l\right), \end{aligned} \quad (25)$$

where  $\{E_l\}_{l=0,1,\dots,n}$  are the energy eigenstates.

This is of course a formal expression; the integration can nevertheless be carried out if we regard (25) as the limit of a similar integral in which  $\lambda$  and  $\nu$  are displaced into the complex along the negative imaginary axis. The integration over  $\mathbb{C}^{n+1}$  then reduces to a  $(2n-2)$ -dimensional Gaussian integral, which is readily performed to yield

$$\Omega(E) = (-i)^{n+1} \pi^n \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{i(\lambda+\nu E)} \prod_{l=0}^n \frac{1}{(\lambda + \nu E_l)}. \quad (26)$$

This is the desired integral representation for the density of states, expressed in terms of the energy eigenvalues.

#### 4.2. Representation in terms of energy eigenvalues

We proceed by evaluating the integration in (26) first in the case where the Hamiltonian has no degenerate eigenvalues. Let us consider the integration in the  $\lambda$  variable first. We observe that there are  $n + 1$  first order poles on the real  $\lambda$ -axis. An application of Cauchy's theorem gives

$$\frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{i(\lambda+\nu E)} \prod_{l=0}^n \frac{1}{(\lambda + \nu E_l)} d\lambda = \sum_{k=0}^n e^{i\nu(E-E_k)} \prod_{l=0, \neq k}^n \frac{1}{\nu(E_l - E_k)}, \quad (27)$$

from which it follows that

$$\Omega(E) = (-1)^n \pi^n \sum_{k=0}^n \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \frac{e^{-i\nu(E_k-E)}}{(-i\nu)^n} \prod_{l=0, \neq k}^n \frac{1}{(E_l - E_k)}. \quad (28)$$

We recognise the  $\nu$ -integration formally as the  $n$ -fold repeated integral of the  $\delta$ -function, defined by the truncated polynomial

$$\delta^{(-n)}(x) = \begin{cases} 0 & (x < 0) \\ \frac{1}{(n-1)!} x^{n-1} & (x \geq 0). \end{cases} \quad (29)$$

As a consequence, the density of states associated with a quantum system having a nondegenerate energy spectrum can be seen to be given by an expression of the form

$$\Omega(E) = (-1)^n \pi^n \sum_{k=0}^n \delta^{(-n)}(E_k - E) \prod_{l=0, \neq k}^n \frac{1}{E_l - E_k}. \quad (30)$$

Equivalently, we can write

$$\Omega(E) = \frac{(-1)^n \pi^n}{(n-1)!} \sum_{k=0}^n \mathbf{1}_{\{E_k \geq E\}} (E_k - E)^{n-1} \prod_{l=0, \neq k}^n \frac{1}{E_l - E_k}. \quad (31)$$

This is our general closed-form expression for the (unnormalised) microcanonical density of states, in the case of a nondegenerate spectrum with a finite number of energy levels. Here  $\mathbf{1}_{\{A\}}$  denotes the indicator function, with the property that  $\mathbf{1}_{\{A\}} = 1$  if  $A$  is true, and  $\mathbf{1}_{\{A\}} = 0$  if  $A$  is false.

Given  $\Omega(E)$ , one can proceed to work out expressions for other thermodynamic variables associated with the equilibrium states of the specified quantum system. In particular, it follows from (6) that the temperature of the system, expressed as a function of the energy, is given by

$$k_B T = - \frac{\sum_{k=0}^n \delta^{(-n)}(E_k - E) \prod_{l=0, \neq k}^n \frac{1}{E_l - E_k}}{\sum_{k=0}^n \delta^{(1-n)}(E_k - E) \prod_{l=0, \neq k}^n \frac{1}{E_l - E_k}}. \quad (32)$$

We note that  $\Omega(E)$  is piecewise polynomial, each polynomial segment being of degree  $n - 1$  in  $E$ . The temperature is given by the ratio of a piecewise polynomial of degree  $n - 1$  to a piecewise polynomial of degree  $n - 2$ .

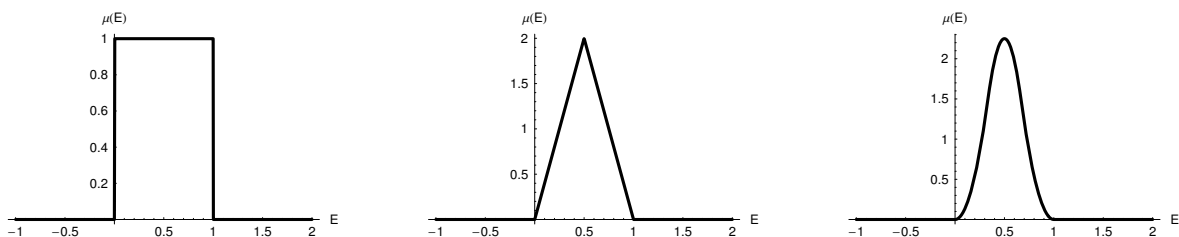
Let us turn now to the degenerate case. We remark that when there are degeneracies in the energy eigenvalues, then associated with any given degenerate eigenvalue there are multiple poles in the integrand of (26). However, because of the relation

$$\frac{1}{(\lambda + \nu E)^a} = \frac{1}{(-\nu)^{a-1}(a-1)!} \left( \frac{d}{dE} \right)^{a-1} \frac{1}{(\lambda + \nu E)}, \quad (33)$$

which holds for any integer  $a \geq 1$ , we can apply the analysis presented above in the case of a nondegenerate spectrum to obtain an expression for the density of states associated with a quantum system having a degenerate spectrum.

More specifically, let  $m$  denote the number of distinct eigenvalues  $E_k$  ( $k = 1, 2, \dots, m$ ), and let  $a_k$  denote the multiplicity associated with the energy  $E_k$ . Thus we have  $\sum_{k=1}^m a_k = n + 1$ . The nondegenerate case is given by  $a_k = 1$  for  $k = 1, 2, \dots, m$ . Otherwise, the spectrum is degenerate. It follows that the density of states associated with a general spectrum is given by

$$\Omega(E) = (-1)^{m+1} \pi^n \prod_{j=1}^m \frac{1}{(a_j - 1)!} \left( \frac{d}{dE} \right)^{a_j-1} \sum_{k=1}^m \delta^{(-n)}(E_k - E) \prod_{l=1, \neq k}^m \frac{1}{E_l - E_k}. \quad (34)$$



**Figure 1.** Density of states as a function of energy  $E$  for systems with two, three, and four nondegenerate energy eigenstates. The functions are evaluated piecewise. For example, in the case of the four-level system with  $E_k/\epsilon = 0, 1, 2, 3$ , the normalised density of states  $\mu(E)$  is zero for  $E \leq 0$  and  $E > 3$ , and is given by three distinct quadratic functions in the intervals  $(0, 1]$ ,  $(1, 2]$ , and  $(2, 3]$ . In general, for an  $(n + 1)$ -level system,  $\mu(E)$  is given by a piecewise combination of polynomials of degree  $n - 1$ , and is at least  $n - 2$  times differentiable for all values of  $E$ . In all cases the area under the function integrates to unity.

In addition to the function  $\Omega(E)$  we find it useful to introduce the related normalised density of states  $\mu(E)$  defined by

$$\mu(E) = \frac{\int_{\Gamma} \delta(H(x) - E) dV}{\int_{\Gamma} dV}. \quad (35)$$

The function  $\mu(E)$  has the property that

$$\int_{-\infty}^{\infty} \mu(E) dE = 1. \quad (36)$$

To calculate the normalisation factor we need the total volume  $V_{\Gamma}$  of the quantum phase space. This is given by

$$V_{\Gamma} = \frac{1}{\pi} \int_{\mathbb{C}^{n+1}} \delta(Z^{\alpha} \bar{Z}_{\alpha} - 1) d^{n+1} Z d^{n+1} \bar{Z}, \quad (37)$$

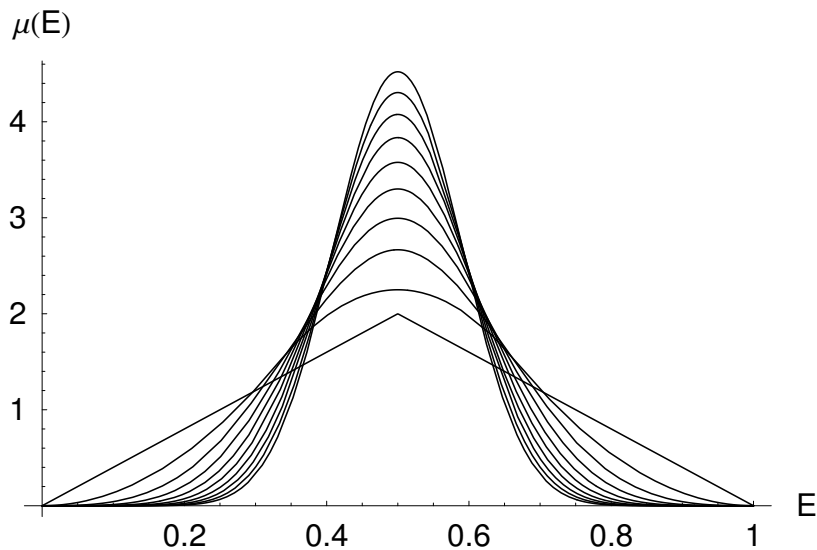
where again the factor of  $\pi$  in the denominator refers to the removal of the superfluous overall phase of the wave function. Making use of the integral representation of the delta-function, we deduce that

$$\begin{aligned}
 V_{\Gamma} &= \frac{1}{\pi} \int_{\mathbb{C}^{n+1}} d^{n+1}Z d^{n+1}\bar{Z} \int_{-\infty}^{\infty} \frac{1}{2\pi} e^{i\lambda(Z^{\alpha}\bar{Z}_{\alpha}-1)} d\lambda \\
 &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{-i\lambda} \int_{\mathbb{C}^{n+1}} e^{i\lambda Z^{\alpha}\bar{Z}_{\alpha}} d^{n+1}Z d^{n+1}\bar{Z} \\
 &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{-i\lambda} \left(-\frac{i\pi}{\lambda}\right)^{n+1} \\
 &= \frac{\pi^n}{n!},
 \end{aligned} \tag{38}$$

where in the last step we have used the identity

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\lambda}}{\lambda^n} d\lambda = \frac{i^n}{(n-1)!}. \tag{39}$$

The formula  $V_{\Gamma} = \pi^n/n!$  is in agreement with the result obtained in [10] by use of other methods. In particular, we note that in the case  $n = 1$  (a two-dimensional Hilbert space) the space of pure states is isomorphic to the geometry of a two-sphere with radius one-half.



**Figure 2.** The normalised density of states  $\mu(E)$  as a function of energy  $E$ . As we increase the density of energy levels in the interval  $[0, 1]$ , the corresponding density of states becomes more sharply distributed around the centre  $E = \frac{1}{2}$ . For these numerical plots we have set  $\epsilon = 1$ . The plots correspond to systems for which the number of energy levels ranges from 3 to 12, and the value of the energy varies over the unit interval. The energy levels are given by  $E_k = k/n$  ( $k = 0, 1, \dots, n$ ), where the number of energy levels is  $n + 1$ .

## 5. Elementary examples with nondegenerate spectrum

### 5.1. Equally spaced energy spectrum

We now proceed to consider in more detail the case of a quantum system whose energy eigenvalues are nondegenerate and equally spaced. In this example we set

$$E_k = \epsilon k, \quad (k = 0, 1, \dots, n), \quad (40)$$

where  $\epsilon$  is a fixed unit of energy. Substituting this expression for  $E_k$  into (30) we obtain

$$\Omega(E) = \frac{(-1)^n}{(n-1)!} \pi^n \epsilon^{-1} \sum_{k \geq E/\epsilon}^n \left(k - \frac{E}{\epsilon}\right)^{n-1} \prod_{l=0, \neq k}^n \frac{1}{(l-k)}. \quad (41)$$

The sum in (41) is understood to extend over nonnegative integral values of  $k$  satisfying  $k \geq E/\epsilon$ . This formula can be simplified further if we note that

$$\prod_{l=0, \neq k}^n \frac{1}{(l-k)} = \frac{1}{(-1)^k k! (n-k)!}. \quad (42)$$

It follows that the density of states associated with a system having an equally-spaced energy spectrum is given by

$$\Omega(E) = \frac{(-1)^n}{(n-1)!} \pi^n \epsilon^{-1} \sum_{k \geq E/\epsilon}^n \frac{(-1)^k (k - E/\epsilon)^{n-1}}{k! (n-k)!}. \quad (43)$$

Finally, dividing this expression by the normalisation factor (38) we obtain the following formula for the normalised density of states:

$$\mu(E) = (-1)^n n \epsilon^{-1} \sum_{k \geq E/\epsilon}^n \frac{(-1)^k (k - E/\epsilon)^{n-1}}{k! (n-k)!}. \quad (44)$$

In Figure 1 we plot  $\mu(E)$  for two, three, and four dimensional Hilbert spaces.

### 5.2. Comparison of state densities when the number of energy levels is increased

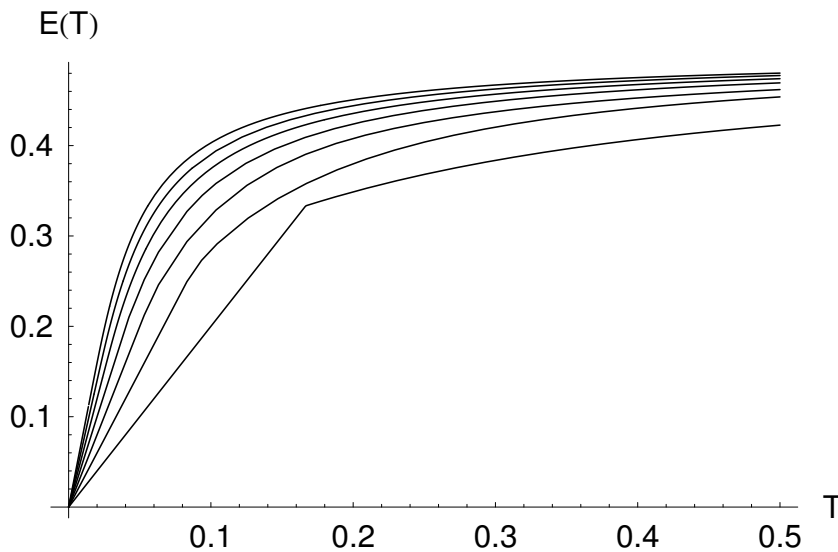
We would like now to study the behaviour of the density of states as we increase the number of energy levels. For this purpose we find it convenient to rescale the energy spectrum so that the range of energy is over a fixed interval. After the application of a suitable such rescaling, the normalised density of states (44) reduces to

$$\mu(E) = (-1)^n n^2 \epsilon^{-1} \sum_{k \geq nE/\epsilon}^n \frac{(-1)^k (k - nE/\epsilon)^{n-1}}{k! (n-k)!}. \quad (45)$$

More precisely, the density (45) is applicable in the case of a quantum system of  $n+1$  equally-spaced energy levels

$$E_k = \epsilon k/n \quad (k = 0, 1, \dots, n), \quad (46)$$

and for which the system energy lies in the fixed range  $E \in [0, \epsilon]$ .



**Figure 3.** The energy  $E(T)$  as a function of the temperature  $T$  in the SQL distribution. The curve that appears to be piecewise almost linear, with lowest energy, corresponds to a four-level system, and we have plotted  $E(T)$  up to the case of a ten-level system, with  $\epsilon = 1$ . Although not shown in the plot, the second root for  $E(0)$  is given by  $E(0) = 1$ , where the function is multi-valued. As  $T$  is reduced from zero,  $E(T)$  decreases monotonically, and changes from  $E = 1$  to  $E = \frac{1}{2}$  as  $T \rightarrow -\infty$ .

In Figure 2 we plot the density of states (45) for a variety of systems with different numbers of energy levels. In Figure 3 we plot the system energy  $E(T)$  for various values of  $n$  as a function of temperature by numerically inverting the relation

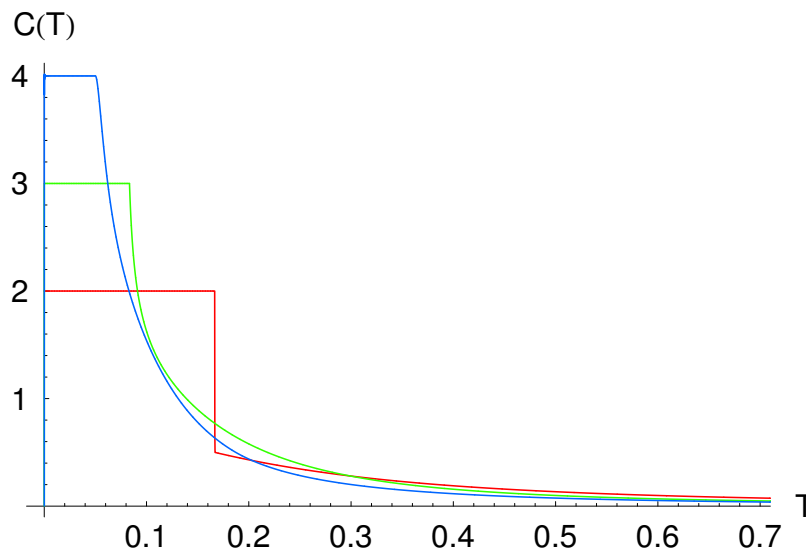
$$k_B T = \frac{\Omega(E)}{\Omega'(E)}, \quad (47)$$

where  $\Omega'(E)$  denotes the derivative of  $\Omega(E)$  with respect to the energy  $E$ . As the temperature increases from zero, the corresponding energy increases monotonically, and asymptotically approaches the value  $E = \frac{1}{2}\epsilon$ . The function  $E(T)$  is multi-valued at  $T = 0$ , where the energy takes the values  $E = 0, \epsilon$ . In the region  $E \in (\frac{1}{2}\epsilon, \epsilon]$  the density of states  $\mu(E)$  is a decreasing function of  $E$ , and thus the corresponding ‘temperature’ is negative (see [23, 24]).

In Figure 4 we plot the specific heat as a function of temperature in the case of the distribution (45) for several different values of  $n$ . The specific heat is defined by the relation  $C(T) = dE/dT$ . In the case of a microcanonical distribution this is given more explicitly by

$$C(T) = \frac{k_B(\Omega')^2}{(\Omega')^2 - \Omega\Omega''}. \quad (48)$$

It is interesting to observe that the specific heat undergoes an abrupt transformation in its behaviour once a certain critical level of the temperature has been reached. This follows from the fact that  $\Omega(E)$  is piecewise polynomial, where in each segment the polynomial is of degree  $n - 1$ . In the case of a four-level system, in particular, there



**Figure 4.** The specific heat  $C(T)$  as a function of the temperature  $T$  in the SQL distribution. The curves show the specific heat for the four-level ( $C(0) = 2$ ), five-level ( $C(0) = 3$ ), and six-level ( $C(0) = 4$ ) systems with a nondegenerate, equally-spaced eigenvalue spectrum spanning a unit interval of energy. The numerical result indicates that these systems exhibit second-order phase transitions at finite temperatures. In particular, the four-level system exhibits a discontinuous drop in the specific heat at a certain critical temperature.

is a discontinuity in the specific heat, which is evident in Figure 4. It should thus be apparent that the kind of quantum gas that we consider exhibits a second-order phase transition. This is perhaps surprising, since no thermodynamic limit has been applied. It is, however, a characteristic feature of the equilibrium states under consideration here that such higher-order phase transitions arise naturally as a consequence of the geometrical structure of the quantum phase space. It is an interesting open question whether any physically realistic low-dimensional systems have as their equilibrium states the distributions we have introduced here. It may be, however, that at low temperatures the quantum gas approximation is invalid, owing to the formation of non-negligible interactions among the constituents in that regime; and hence one might not generally see the specific heats implied by the model at low temperature.

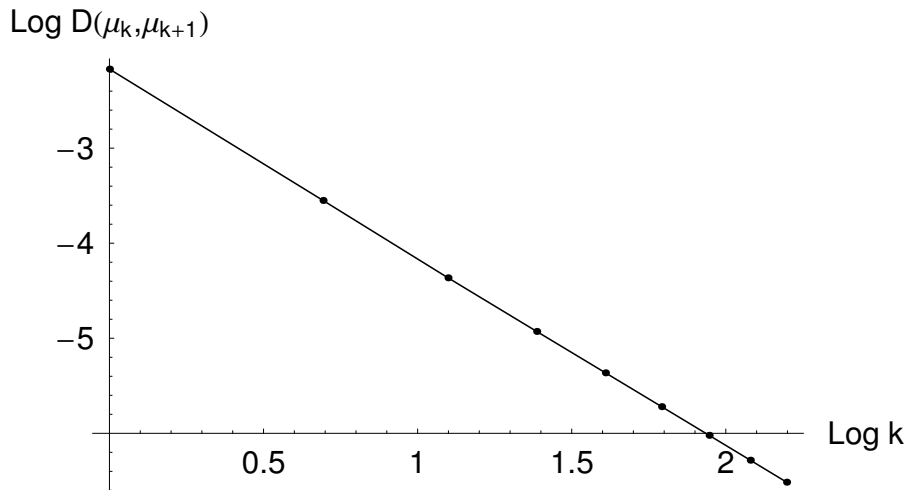
### 5.3. Limiting distribution

The numerical results shown in Figure 2 indicate that as we increase the number of energy levels in the system with spectrum (46) the density of states becomes more and more peaked at the intermediate energy  $E = \frac{1}{2}\epsilon$ . This does not, as such, imply that the density function converges in this limit. Therefore, to obtain better numerical evidence we consider the separation of a pair of normalised state densities associated with  $n$ -level and  $(n + 1)$ -level systems for a range of values for  $n$ , and study whether the separation decreases as we increase  $n$ . There are various standard measures that one can use to

study the separation of a pair of density functions, such as the relative entropy or the Bhattacharyya distance. Here we make use of a closely related measure given by

$$D(\mu_m, \mu_n) = \left\| \sqrt{\mu_m(E)} - \sqrt{\mu_n(E)} \right\|, \quad (49)$$

known as the Hellinger distance. For clarity we let  $\mu_n(E)$  denote the density of states associated with an  $(n + 1)$ -level system.



**Figure 5.** The Hellinger distance  $D(\mu_n, \mu_{n+1})$  between two consecutive state densities for  $n = 1, 2, \dots, 9$ . The plot is presented on a logarithmic scale. We find that the logarithms of the distances lie very nearly on a straight line with gradient of  $-2$ , indicating that the separation of the densities decays quadratically with an increasing number of energy levels. For each value of  $n$ , the quantum system under consideration has  $n + 1$  energy levels that are equally spaced over a unit interval of energy.

The result of the numerical analysis of (49) is shown in Figure 5, which indicates that the relative separation of  $\mu_n(E)$  and  $\mu_{n+1}(E)$  decreases quadratically in  $n$ . We conclude on the basis of the numerical evidence that the density of states is likely to converge.

#### 5.4. Other spectral structures

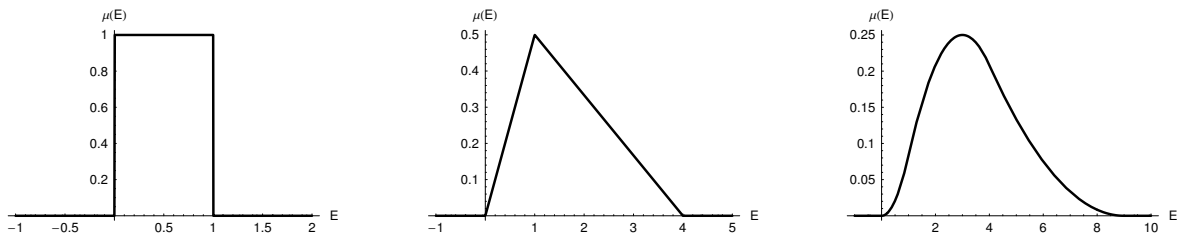
In the examples considered above we analysed linear spectral structures. In this section we investigate nondegenerate systems having other energy growth rates. We start with the case of a system whose energy grows quadratically, so  $E_k = \epsilon k^2$ . In this case we make use of the relation

$$\prod_{l=0, \neq k}^n \frac{1}{l^2 - k^2} = \prod_{l=0, \neq k}^n \frac{1}{(l+k)(l-k)} = \frac{2(-1)^k}{(n+k)!(n-k)!}, \quad (50)$$

and substitute this in formula (30) to obtain

$$\mu(E) = 2n(-1)^n \epsilon^{-1} \sum_{k=0}^n \mathbf{1}_{k^2 \geq E/\epsilon} \frac{(-1)^k (k^2 - \frac{E}{\epsilon})^{n-1}}{(n+k)!(n-k)!}. \quad (51)$$

As one might expect, the functions given by (51) have characteristics similar to those of the previous example. For each value of  $n$  we obtain a curve  $\mu(E)$  which is specified by  $n + 2$  polynomials of degree  $n - 1$ . The function is continuous and is at least  $n - 2$  times differentiable for all  $E$ . The first three examples are plotted in Figure 6. As the plots indicate, the density functions in the current examples are no longer symmetric around the intermediate energy  $\frac{1}{2}(E_{\min} + E_{\max})$ , in contrast to the case of linear energy growth.



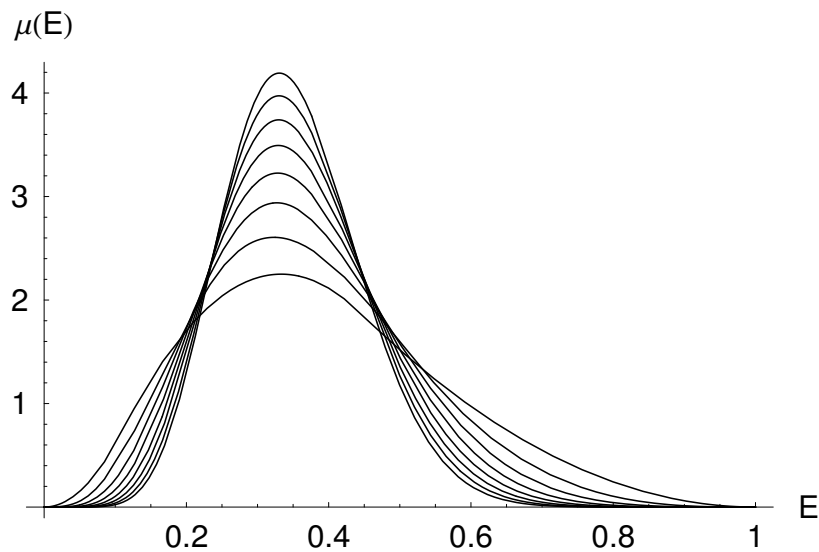
**Figure 6.** The density of states  $\mu(E)$  for  $(n + 1)$ -level systems with  $n = 1, 2, 3$  in the case of a Hamiltonian with a quadratically growing energy spectrum  $E_k = \epsilon k^2$ . For the plot we have set  $\epsilon = 1$ . Unlike the example with a linear, equally-spaced spectrum, the density of states is not symmetric.

As in the previous example, we can rescale the energy spectrum in such a way that we can directly compare the behaviours of the densities as we increase the number of energy levels. For each  $n$ , the modified spectrum is then given by  $E_k = \epsilon k^2/n^2$  ( $k = 0, 1, \dots, n$ ). The result is shown in Figure 7. We observe that the density of states becomes more peaked as we increase the number of energy levels. However, the location of the peak is no longer at  $E = \frac{1}{2}\epsilon$ , but rather is closer to  $E = \frac{1}{3}\epsilon$ .

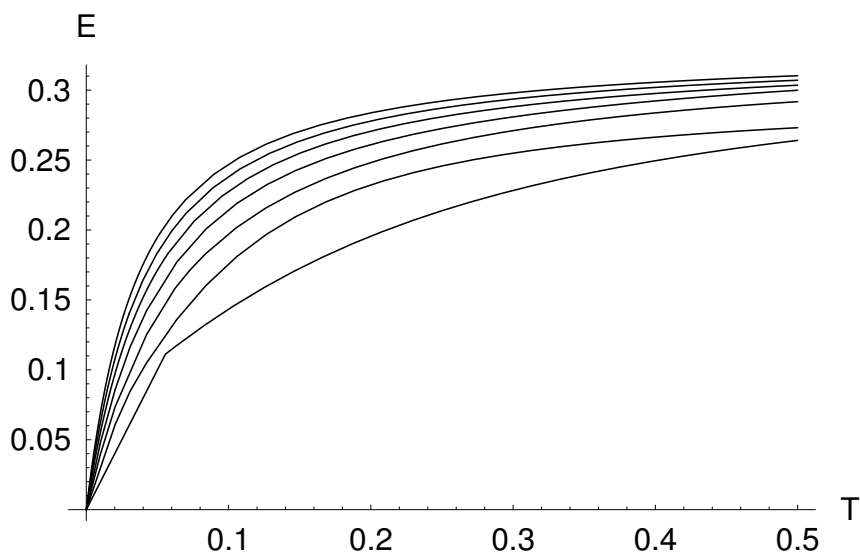
As a consequence of the skewed form of the distribution, the range of energy for which the derivative of  $\mu(E)$  with respect to  $E$  remains positive is reduced. This implies that the range of energy associated with positive temperature is reduced from what it was in the example of a linear spectrum. In Figure 8, we plot the temperature dependence of the energy. As the temperature is increased, the energy grows monotonically and reaches a value around  $\frac{1}{3}\epsilon$ . The remaining values of the energy are associated with negative temperatures.

We have examined systems having a linear energy growth and a quadratic energy growth. In the linear case the resulting microcanonical distribution is symmetric around its centre, while in the quadratic case the peaks of the distributions have shifted to the left with smaller energies. This leads to the question of what happens to the density of states associated with systems having other spectral structures.

In the case of a system with a countably infinite number of degrees of freedom (and thus an infinite number of discrete energy levels), the energy spectrum cannot grow more rapidly than quadratically in the number of energy levels. However, in the case of a finite system there is in principle no limitation on how fast the energy can grow. Therefore, we study the behaviour of the density of states associated with systems



**Figure 7.** The density of states  $\mu(E)$  associated with a system having the spectrum  $E_k = k^2/n^2$ . The value of  $k$  ranges over  $k = 0, 1, \dots, n$ . The unit of energy is  $\epsilon = 1$ . Here we plot  $\mu(E)$  for  $n = 4, 5, \dots, 11$ . Numerical studies show that the peaks of the distributions are located at approximately  $E = \frac{1}{3}$ .



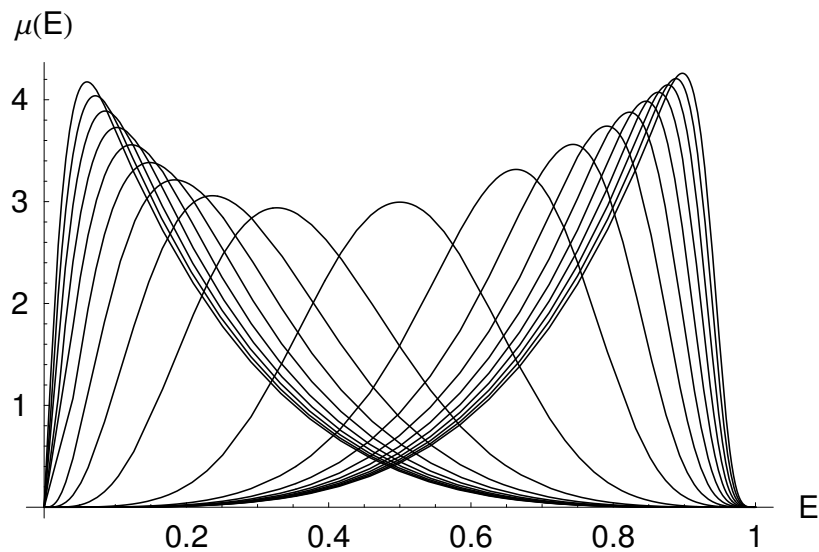
**Figure 8.** The energy  $E(T)$  as a function of temperature  $T$  in the case of a system having a quadratic energy spectrum. The plots correspond to a set of 5, 6,  $\dots$ , 11-level systems. Although not shown in the plot, the energy is multi-valued at  $T = 0$  so that  $E(T) \rightarrow 0$  as  $T \rightarrow 0^+$  and  $E(T) \rightarrow 1$  as  $T \rightarrow 0^-$ . The accessible range of energy is given by  $0 \leq E \lesssim \frac{1}{3}$ .

having the following two families of spectral structures:

$$E_k = \epsilon k^m / n^m \quad \text{and} \quad E_k = \epsilon k^{1/m} / n^{1/m}, \quad (52)$$

for  $k = 0, 1, 2, \dots, n$  and  $m = 1, 2, 3, \dots$ . In the first family the growth of the energy is enhanced as  $k$  is increased, while in the second family the growth of the energy is

suppressed. Various densities of states associated with systems having spectra of the form (52) are computed numerically and plotted in Figure 9. The result shows that as the rate of growth is increased, the location of the peak of  $\mu(E)$  becomes smaller, whereas when the rate of energy growth is suppressed, the peak of  $\mu(E)$  increases. In particular, if we set  $\epsilon = 1$  we find that the peak of  $\mu(E)$  for the system with energy  $E_k = k^m/n^m$  is located approximately at  $E \sim (m + 1)^{-1}$ , while the peak of  $\mu(E)$  for the system with energy  $E_k = k^{1/m}/n^{1/m}$  is located approximately at  $E \sim 1 - (m + 1)^{-1}$ . When  $m \ll 1$ , the values of the energy that are accessible in equilibrium become negligible when  $E_k = k^m/n^m$ , whereas if  $E_k = k^{1/m}/n^{1/m}$  then virtually all values of  $E \in [0, 1]$  are accessible.



**Figure 9.** The density of states  $\mu(E)$  associated with systems having the spectra  $E_k = k^m/n^m$  and  $E_k = k^{1/m}/n^{1/m}$ , for  $m = 1, 2, \dots, 10$ . In the former case the peak of  $\mu(E)$  shifts to the left, while in the latter case the peak shifts to the right. The cases  $E_k = k^m/n^m$  and  $E_k = k^{1/m}/n^{1/m}$  are close to being symmetrically related to one another around  $E = \frac{1}{2}$ . In all examples the number of energy levels is set to six, so  $k = 0, 1, \dots, 5$ .

## 6. Discussion

It should be evident from the analysis carried out in this paper that a more or less complete theory of the quantum microcanonical distribution can be formulated in a way that respects the natural Hamiltonian structure of the quantum state space. The resulting density matrix differs from that of the more familiar treatments, and as a consequence it is probably correct to call our approach a new theory of quantum statistical mechanics—in any event, we stress that it is not merely a reformulation of the ‘standard’ theory in a geometrical language.

The only approach to the standard theory, of which we are aware, that is pursued in a manner sufficiently geometrical in character that it allows for a direct comparison

with our method is that of Khinchin [16]. Khinchin eschews the notion of ensembles (as do we, in this paper), and defines the microcanonical distribution only for the energy levels of the quantum system under consideration. He assumes a discrete spectrum, and has in mind the situation where the levels can be highly degenerate. The space of pure states that are energy eigenstates with the given (degenerate) energy level then constitute a submanifold of the space of pure states, and that submanifold is what Khinchin regards as the energy surface. If the multiplicity of the level is  $m$ , the real dimension of the energy surface is  $2m - 2$ . He then goes on to show that if a uniform distribution is put on such an energy surface, and if one averages the expectation value of an observable with respect to this uniform distribution (this involves a nontrivial calculation), then the result is the same as the expectation of the given observable with respect to the ‘standard’ microcanonical density matrix for the given energy level. Khinchin’s argument is perhaps the most cogent available in support of the standard microcanonical density matrix. It does not, however, lead in any natural way to a smooth parametric family of states for general values of  $E$  (i.e. for values other than eigenvalues); as a consequence the notion of temperature is not well defined from first principles, and has to be introduced instead in a rather *ad hoc* way via the canonical distribution. The situation is thus in sharp contrast with the methodology of classical statistical mechanics, where the microcanonical distribution plays a foundational role.

In the theory that we have proposed, the symplectic microcanonical distribution (we add the word ‘symplectic’ to stress its connection with the geometry of the state space, and to distinguish it from the standard distribution) is well defined for all admissible values of the total energy, and hence is more suitable as a basis for developing statistical mechanics in general. In particular, the generic energy surface is a real hypersurface of codimension one in the quantum phase space, just as it is in the classical theory. As a consequence the temperature and the specific heat are generally both well defined for this distribution, and are given by the usual thermodynamic relations. On the other hand, the fact that the underlying system is quantum mechanical makes its impact in a number of distinct ways. Since the quantum systems we consider here are finite-dimensional, with a finite set of energy levels, it is not surprising that the higher energy states have negative absolute temperatures; indeed, this is exactly what one would expect from Ramsey’s theory [23, 24] of negative temperature. Perhaps the biggest surprise is the appearance of second-order phase transitions. The simplest example of this kind of ‘symplectic’ phase transition occurs in the case of a four-level system with equally-spaced energy levels. The density of states for this system is differentiable for all values of the energy, and the corresponding temperature is therefore continuous in  $E$ ; but the heat capacity has a discontinuity at a certain finite critical value of the temperature. The critical value of the temperature is that associated with the second energy level, at which point there is an abrupt drop in the heat capacity. In the case of a system with a larger number of energy levels, the same phenomenon persists, the only difference being that the drop in the heat capacity is somewhat less precipitate. In fact, the drop remains quite steep, albeit no longer strictly discontinuous.

The conventional wisdom in statistical mechanics is that phase transitions are impossible in models for finite-dimensional quantum systems; that only in the thermodynamic limit can such phenomena develop. The present investigation, however, shows a gap in the reasoning behind that line of thought. The conventional approach has been pursued almost entirely in the context of the canonical distribution, where indeed—owing to the analytic dependence of the distribution function on the temperature—phase transitions are ruled out without the invocation of the thermodynamic limit. On the other hand, the standard microcanonical distribution does not lead to an unambiguous definition of the relevant thermodynamic variables—unless one takes the thermodynamic limit (as discussed, e.g., in [11]). The present paper shows, however, that once a suitable definition is given for the microcanonical distribution, then owing to the nonanalytic nature of the density of states one can expect to see a variety of interesting physical phenomena emerging in models for the equilibrium behaviour of finite-dimensional quantum systems.

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